

10/513699

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NEWS 16 JUN 01 CAS REGISTRY Source of Registration (SR) searching enhanced on STN

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STRUCTURE FILE UPDATES: 21 JUN 2009 HIGHEST RN 1159253-26-5
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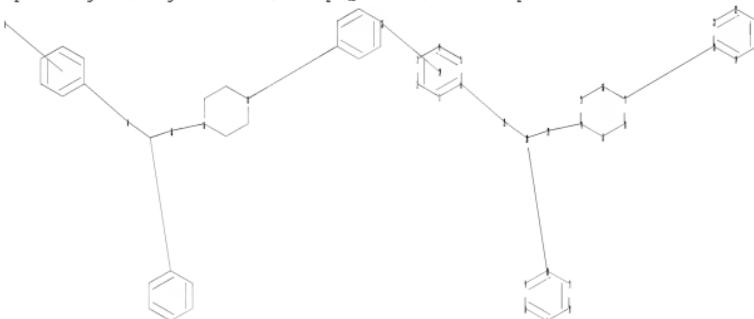
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10/513699

chain nodes :
25 26 27 28
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-28 14-27 17-20 25-28 27-28
ring bonds :
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exact/norm bonds :
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exact bonds :
10-28
normalized bonds :
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20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:Atom

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=> s 11 full
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FULL SCREEN SEARCH COMPLETED - 11045 TO ITERATE

100.0% PROCESSED 11045 ITERATIONS 88 ANSWERS
SEARCH TIME: 00.00.01

L2 88 SEA SSS FUL L1

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FILE LAST UPDATED: 21 Jun 2009 (20090621/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

Cplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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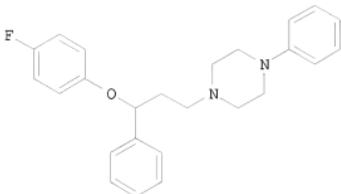
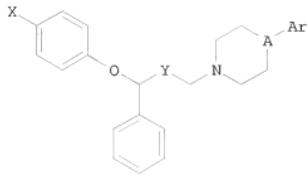
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=> s 12 full
L3          2 L2

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10/513699

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103625 CAPLUS
DOCUMENT NUMBER: 143:387060
TITLE: Preparation of piperazine or piperidine derivatives as serotonin reuptake inhibitors
INVENTOR(S): Pinney, Kevin G.; Miranda, Maria Graciela; Dorsey, James Michael
PATENT ASSIGNEE(S): Baylor University, USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005094896	A2	20051013	WO 2005-US10356	20050328
WO 2005094896	A3	20070503		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AP, EA, EP, OA				
EP 1732610	A2	20061220	EP 2005-730778	20050328
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US 20080132514	A1	20080605	US 2007-594105	20070921
PRIORITY APPLN. INFO.:			US 2004-557069P	P 20040326
			WO 2005-US10356	W 20050328
OTHER SOURCE(S):	CASREACT 143:387060; MARPAT 143:387060			
GI				



AB Title compds. I [X = F or CF₃; Y = (CH₂)_n; n = 0-1; A = N or C; Ar = aryl] and their pharmaceutically acceptable salts, are prepared and disclosed as serotonin reuptake inhibitors. Thus, e.g., II was prepared by reduction of 1-phenyl-3-(4-phenyl-piperazin-1-yl)-propan-1-ol (preparation given) using sodium borohydride followed by coupling with 4-fluorophenol. The ability of I to inhibit [³H]5-HT uptake was evaluated using liquid scintillation spectroscopy and it was revealed that selected compds. of the invention possessed IC₅₀ values in the range of 1.45 up to 9.56 μM. I as serotonin reuptake inhibitors should prove useful in the treatment of depression. Pharmaceutical composition comprising I are disclosed.

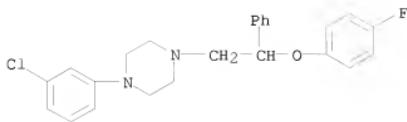
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 691872-62-5P 691872-64-7P 691872-66-9P
 866548-21-2P 866548-22-3P 866548-24-5P
 866548-25-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of piperazine or piperidine derivs. as serotonin reuptake inhibitors)

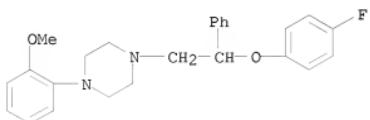
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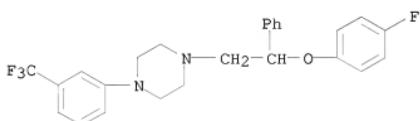
10/513699



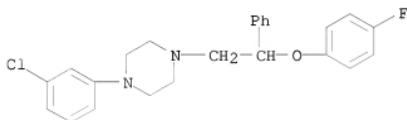
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(CA INDEX NAME)



RN 691872-60-3 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 691872-62-5 CAPLUS
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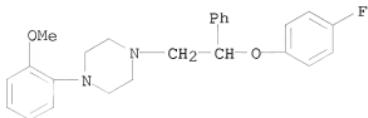


● HCl

RN 691872-64-7 CAPLUS

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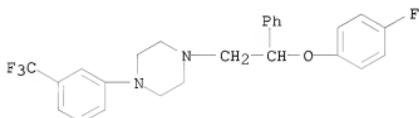
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RN 691872-66-9 CAPLUS

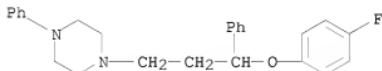
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• HGL

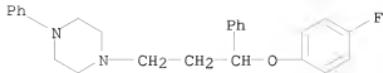
RN 866548-21-2 CAPLUS

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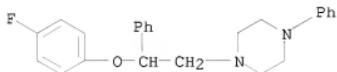
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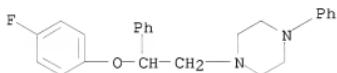


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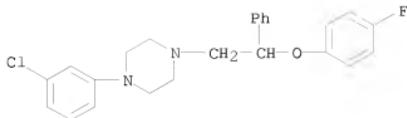


RN 866548-25-6 CAPLUS
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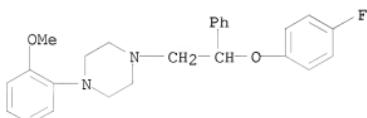
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L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2004:170822 CAPLUS
 DOCUMENT NUMBER: 140:417233
 TITLE: Synthesis and biological evaluation of
 2-(4-fluorophenoxy)-2-phenyl-ethyl piperazines as
 serotonin-selective reuptake inhibitors with a
 potentially improved adverse reaction profile
 AUTHOR(S): Dorsey, James M.; Miranda, Maria G.; Cozzi, Nicholas
 V.; Pinney, Kevin G.
 CORPORATE SOURCE: Department of Chemistry and Biochemistry and The
 Center for Drug Discovery, Baylor University, Waco,
 TX, 76798-7348, USA
 SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(6),
 1483-1491
 PUBLISHER: CODEN: BMECEP; ISSN: 0968-0896
 DOCUMENT TYPE: Elsevier Ltd.
 LANGUAGE: Journal
 OTHER SOURCE(S): English
 CASREACT 140:417233
 AB Three new 2-(4-fluorophenoxy)-2-phenyl-Et piperazines,
 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-piperazine,
 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-piperazine, and
 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(3-trifluoromethylphenyl)-
 piperazine, modeled after the potent antidepressant fluoxetine and coupled
 with several functionalized piperazines, have been prepared by chemical
 synthesis as selective serotonin reuptake inhibitors (SSRIs) with a
 potentially improved adverse reaction profile. Typical SSRIs, although
 very effective in the treatment of depression, still face the troublesome
 side effect of sexual dysfunction. A number of pharmacol. agents—notably,
 drugs in the piperazine class—have been used to reverse SSRI-induced
 sexual dysfunction, and evidence for developing an improved SSRI by
 coupling a fluoxetine congener with the pharmacophore of a reversal agent
 holds promise. Preliminary data indicates that the hydrochloride (HCl)
 salts of piperazines exhibit single-site binding at the site of the
 serotonin reuptake transporter (SERT). However, each of the three compds.
 are much less potent than typical SSRIs, showing micromolar (μ M)
 affinity for the SERT with IC₅₀ values of 1.45 μ M, 3.27 μ M, and 9.56
 μ M, resp. Further biol. evalution of piperazine compds. is needed
 before definitive conclusions can be made with regard to each compound's
 potential for use as an SSRI-type candidate which is devoid of sexual side
 effects. Nevertheless, the initial findings are quite encouraging, thus
 lending credence to the idea of hybridizing an SSRI congener with that of
 the pharmacophore of an agent known to reverse or treat SSRI-induced
 sexual dysfunction.
 IT 691872-62-5P 691872-64-7P 691872-66-9P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (synthesis and structure-activity relationship of
 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake
 inhibitors with a potentially improved adverse reaction profile)
 RN 691872-62-5 CAPLUS
 CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-,
 hydrochloride (1:1) (CA INDEX NAME)



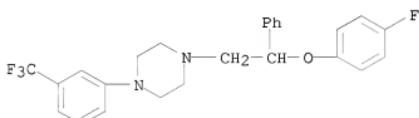
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RN 691872-64-7 CAPLUS
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● HCl

RN 691872-66-9 CAPLUS
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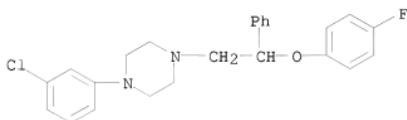


● HCl

IT 691872-56-7P 691872-58-9P 691872-60-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthesis and structure-activity relationship of
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 inhibitors with a potentially improved adverse reaction profile)
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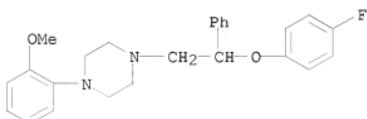
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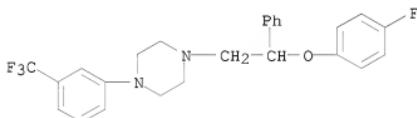
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RN 691872-60-3 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT:

14

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L3 FILE 'CPLUS' ENTERED AT 15:53:50 ON 22 JUN 2009
2 S L2 FULL

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